Pentyl acetate

628-63-7 | DTXSID1027263

## Model Performance

| Model | Data |
|---|---|

### Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|---|---|---|---|---|---|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.72 | 51.8 | 0.74 | 50.3 | 0.73 | 52.7 |

## Model Results

**Predicted value:** -83.2 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 9.88e-01

**Confidence level:** 7.98e-01

## Nearest Neighbors from the Training Set

Image not found
Pentyl acetate
**Measured:** -70.8
**Predicted:** -83.2

Image not found
Ethyl valerate
**Measured:** -91.2
**Predicted:** -83.8

Image not found
Butyl propionate
**Measured:** -89.0
**Predicted:** -84.2

Image not found
Butanoic acid, propyl ester
**Measured:** -95.2
**Predicted:** -84.3

Image not found
Methyl hexanoate
**Measured:** -71.0
**Predicted:** -82.6